Runge-Kutta

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Recall local truncation error $\tau_{i+1}(h) := \frac{1}{h}\left(y_{i+1} - (y_i + h\,\phi(t_i, y_i))\right)$

for the method $w_{i+1} = w_i + h\phi(t_i, w_i)$.

Euler's method has $\tau(h) = O(h)$. Higher-order methods do better, e.g., $O(h^2)$

We saw higher-order Taylor methods based on Taylor expansions of f

(recall: our IVP is $y' = f(t,y)$, $y(a) = y_0$, $t \in [a,b]$)

This lecture: a better way to get higher-order methods

Background: Taylor's Thm in 2D

Thm 5.13 Suppose $f(t,y)$ and all its partial derivatives of order $\le n+1$ are continuous on $D = \{ (t,y) : a \le t \le b,\ c \le y \le d \}$, and let $(t_0, y_0) \in D$. Then $\forall\ (t,y) \in D$, $\exists\ \xi$ between t and t_0 and $\exists\ \mu$ between y and y_0 with

$$f(t,y) = \underbrace{P_n(t,y)}_{\text{Taylor polynomial}} + \underbrace{R_n(t,y)}_{\text{error / remainder}}$$

where

$$P_n(t,y) = \underbrace{f(t_0,y_0)}_{0^{th}\text{ order}} + \underbrace{(t-t_0)\frac{\partial f}{\partial t}(t_0,y_0) + (y-y_0)\frac{\partial f}{\partial y}(t_0,y_0)}_{1^{st}\text{ order terms}}$$

$$+ \underbrace{\frac{(t-t_0)^2}{2!}\frac{\partial^2 f}{\partial t^2}(t_0,y_0) + (t-t_0)(y-y_0)\frac{\partial^2 f}{\partial t\,\partial y}(t_0,y_0) + \frac{(y-y_0)^2}{2!}\frac{\partial^2 f}{\partial y^2}(t_0,y_0)}_{2^{nd}\text{ order terms}}$$

Recall $\binom{n}{j} = \frac{n!}{(n-j)!\,j!}$

$$+ \cdots + \underbrace{\frac{1}{n!}\sum_{j=0}^{n}\binom{n}{j}(t-t_0)^{n-j}(y-y_0)^j \frac{\partial^n f}{\partial t^{n-j}\partial y^j}(t_0,y_0)}_{n^{th}\text{ order terms}}$$

and the remainder term is

$$R_n(t,y) = \frac{1}{(n+1)!}\sum_{j=0}^{n+1}\binom{n+1}{j}(t-t_0)^{n+1-j}(y-y_0)^j \frac{\partial^{n+1} f}{\partial t^{n+1-j}\partial y^j}(\xi,\mu)$$

Idea of Runge-Kutta

Carl Runge 1856-1927, Martin Kutta 1867-1944

A family of methods, not a single method

$$y(t+h) = y(t) + h\cdot \underbrace{y'(t)}_{\substack{f(t,y)\\ \text{via ODE}}} + \frac{h^2}{2}\underbrace{y''(t)}_{f'(t,y)} + O(h^3)$$

So our 1^{st} order Taylor method (Euler's method) is $\phi(t,y) = f(t,y)$

$$w_{i+1} = w_i + h\,\phi(t_i, w_i) \quad \Big\}\ \text{Generic form of one-step methods (of which RK belongs)}$$

and $\underbrace{2^{nd}\text{ order Taylor method}}_{T^{(2)}}$ is $\underbrace{\phi(t,y)}_{T^{(2)}} = f(t,y) + h/2\, f'(t,y)$

etc.

Focus on $T^{(2)}$ for now. We'd like to avoid calculating $f'(t,y)$.

Let's approximate it with Taylor Series! (if you haven't noticed yet, that's the theme of this class)

How many terms to keep in the Taylor Series?

We already have a $O(h^2)$ error in ϕ, so let's keep at some amount

It gets a bit messy.

Recall chain rule $f'(t,y) := \frac{d}{dt}f(t,y) = \frac{\partial}{\partial t}f(t,y) + \frac{\partial}{\partial y}f(t,y)\cdot \overbrace{\frac{dy}{dt}}^{=y'=f}$

so

$$T^{(2)}(t,y) = \overbrace{f(t,y)}^{①} + \overbrace{\frac{h}{2}\frac{\partial f}{\partial t}(t,y)}^{②} + \overbrace{\frac{h}{2}\frac{\partial f}{\partial y}(t,y)\cdot f(t,y)}^{③}$$

Idea: can we find a, α and β such that

$$T^{(2)}(t,y) = \underbrace{a\cdot f(t+\alpha, y+\beta)}_{\text{Taylor expand (2D) about } f(t,y)} + O(h^2)\ ?$$

match

$$a\cdot f(t+\alpha, y+\beta) = a\left(\overbrace{f(t,y)}^{①} + \overbrace{\alpha\frac{\partial f}{\partial t}(t,y)}^{②} + \overbrace{\beta\frac{\partial f}{\partial y}(t,y)}^{③}\right)$$

$$+\ a R_1(t+\alpha, y+\beta)$$

So matching terms

① $\Rightarrow$ $\boxed{a=1}$

② $\Rightarrow$ $a\alpha = h/2$ so $\boxed{\alpha = h/2}$

③ $\Rightarrow$ $a\beta = h/2\cdot f(t,y)$ so $\boxed{\beta = h/2\, f(t,y)}$

and if $f(t,y)$ and all of its partial derivatives up to degree ≤ 2 are bounded, then $R_1(\ldots) = O(h^2)$ ✓

We just derived the

Midpoint Method, a.k.a. **Improved Euler** (an example of a Runge-Kutta method)

$$w_0 = y_0$$

$$w_{i+1} = w_i + h \cdot f\left(t_i + \frac{h}{2},\ w_i + \frac{h}{2} f(t_i, w_i)\right)$$

still "single step" but we call it "multistage"

Another way to write it:

Given w_i,
$$k_1 = h f(t_i, w_i)$$
$$k_2 = h f(t_i + h/2,\ w_i + \tfrac{1}{2} k_1)$$
$$w_{i+1} = w_i + k_2$$

⚠ Twice the cost per iteration, compared to Euler, but usually definitely worth it.

General form of Runge-Kutta methods

we can generalize above, adding more parameters to get higher-orders RK methods. All s-step explicit Runge-Kutta methods can be described by their "Butcher array"

$$\begin{array}{c|ccccc}
0 & & & & & \\
c_1 & a_{11} & & & & \\
c_2 & a_{21} & a_{22} & & & \\
\vdots & \vdots & \vdots & \ddots & & \\
c_{s-1} & a_{s-1,1} & a_{s-1,2} & \cdots & a_{s-1,s-1} & \\
\hline
 & b_1 & b_2 & \cdots & b_{s-1} & b_s
\end{array}$$

meaning

$$k_1 = h f(t_i, w_i)$$
$$k_2 = h f(t_i + c_1 h,\ w_i + a_{11} k_1)$$
$$k_3 = h f(t_i + c_2 h,\ w_i + a_{21} k_1 + a_{22} k_2)$$
$$\vdots$$
$$k_s = h f(t_i + c_{s-1} h,\ w_i + a_{s-1,1} k_1 + \ldots)$$
$$w_{i+1} = w_i + b_1 k_1 + b_2 k_2 + \ldots + b_s k_s$$

Ex Improved Euler

$$k_1 = h f(t_i, w_i)$$
$$k_2 = h f(t_i + h/2,\ w_i + \tfrac{1}{2} k_1)$$
$$w_{i+1} = w_i + k_2$$

$c_1 = 1/2$, $a_{11} = 1/2$

($b_2 = 1$, $b_1 = 0$)

Butcher array

$$\begin{array}{c|cc}
0 & & \\
1/2 & 1/2 & \\
\hline
 & 0 & 1
\end{array}$$

Ex Modified Euler (also a 2-stage, 2nd order method)

Our book defines it as $w_{i+1} = w_i + \frac{h}{2}\left[f(t_i, w_i) + f(t_{i+1}, w_i + h f(t_i, w_i))\right]$

$$= w_i + \frac{1}{2} \underbrace{h f(t_i, w_i)}_{K_1} + \frac{1}{2} \underbrace{h f(t_i + h, w_i + h \underbrace{f(t_i, w_i)}_{K_1})}_{K_2}$$

$b_1 = 1/2$ $\quad b_2 = 1/2$ $\quad c_1 = 1$ $\quad a_{11} = 1$

So the Butcher array is

$$\begin{array}{c|cc} 0 & & \\ 1 & 1 & \\ \hline & 1/2 & 1/2 \end{array}$$

Another ex. of a 2-stage, 2nd order method is Heun's 2-stage method

not the same as our book's 3-stage, 3rd order Heun's method.

$$\begin{array}{c|cc} 0 & & \\ 2/3 & 2/3 & \\ \hline & 1/4 & 3/4 \end{array}$$

← note: b_i's always sum to 1

(for consistency)

There are systematic ways to derive these, but complicated and... it only has to be done once. We can just use them

The zoo of RK methods: higher-order RK, and which ones to use?